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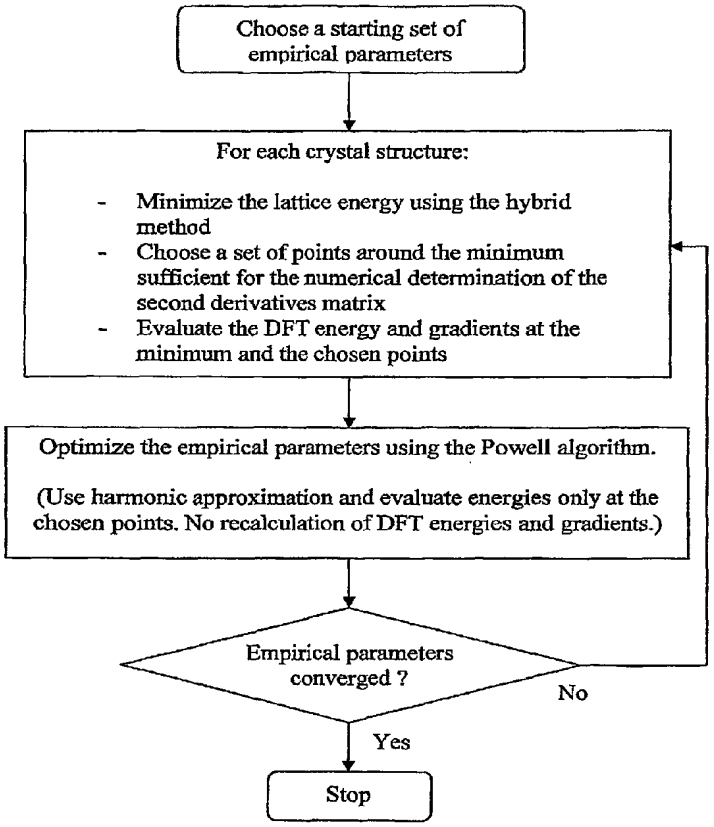
(54) Title: METHOD FOR ENERGY RANKING OF MOLECULAR CRYSTALS USING DFT CALCULATIONS AND EMPIRICAL VAN DER WAALS POTENTIALS



(57) Abstract: The invention refers to a method for the accurate determination of van der Waals parameters for high-precision determination of crystal structures and/or energies, comprising the steps of: numerically simulating at least one crystal structure based on density functional theory (DFT) calculations combined with a potential energy term representing van der Waals interactions; providing reference data containing accurate information about said at least one crystal structure; defining a deviation function (F) quantifying a deviation between said reference data and said at least one simulated crystal structure; fitting at least one parameter of said van der Waals potential term in such a way as to minimize said deviation function (F); and obtaining the accurate van der Waals parameters from the best fit. The invention furthermore deals with a hybrid method for the accurate van der Waals parameters from the best fit. The invention furthermore deals with a hybrid method for the accurate determination of crystal structures and/or energies based on such a parameter determination as well as the general application of such a hybrid method to the energy ranking of polymorphic crystal structures.

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